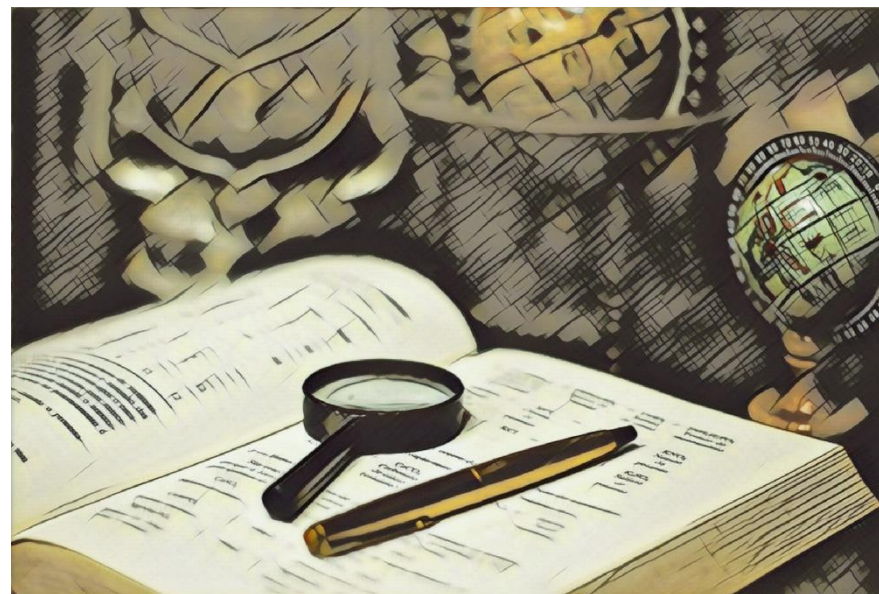


Como Usar o PubChem

Prof. Dr. Walter F. de Azevedo Jr.



O PubChem (<https://pubchem.ncbi.nlm.nih.gov/>) é uma base de dados sobre a estrutura de moléculas. No PubChem há informações completas sobre a estrutura, perfil físico-químico e características farmacológicas de milhões de moléculas. Aqui está descrito como usar esta ferramenta e exemplos de como obter informações químicas armazenadas no PubChem.



No estudo de fármacos é comum lidarmos com reagentes diversos para o preparo de soluções. Informações sobre parâmetros físico-químicos e biológicos podem ser encontradas em base de dados como o [PubChem](https://pubchem.ncbi.nlm.nih.gov/) (<https://pubchem.ncbi.nlm.nih.gov/>). O PubChem permite uma busca por reagentes específicos, abaixo temos a página de entrada do PubChem (acesso em 06 de junho de 2020).

The screenshot shows the PubChem website homepage. At the top, there is a navigation bar with the NIH logo and the text "U.S. National Library of Medicine National Center for Biotechnology Information". Below this is the PubChem logo and a navigation menu with links for "About", "Blog", "Submit", and "Contact". A link for "PubChem Periodic Table and Element pages" with a "Read More" button is also present. The main content area features a large blue banner with the text "Explore Chemistry" and "Quickly find chemical information from authoritative sources". Below the banner is a search bar with a magnifying glass icon. Underneath the search bar, there are several search suggestions: "Try aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)4/h1-2H3". At the bottom of the page, there are four icons representing different functions: "Draw Structure" (a pencil and a chemical structure), "Upload ID List" (an upward arrow), "Browse Data" (a grid of squares), and "Periodic Table" (a grid of dots representing a periodic table).

Para ilustrar, vamos considerar uma busca pelo cloreto de sódio (NaCl) no PubChem. Para a busca por substâncias no PubChem, usaremos o nome em inglês, no caso “sodium chloride”.

The image shows a screenshot of the PubChem website homepage. The browser address bar displays "pubchem.ncbi.nlm.nih.gov". The page header includes the NIH logo and the text "U.S. National Library of Medicine National Center for Biotechnology Information". The main navigation bar features the PubChem logo and links for "About", "Blog", "Submit", and "Contact". A link for "PubChem Periodic Table and Element pages" is also visible. The main content area has a large blue background with the text "Explore Chemistry" and "Quickly find chemical information from authoritative sources". Below this is a search bar with a magnifying glass icon. Underneath the search bar, there are several search suggestions: "Try aspirin", "EGFR", "C9H8O4", "57-27-2", "C1=CC=C(C=C1)C=O", and "InChI=1S/C3H6O/c1-3(2)4/h1-2H3". At the bottom of the page, there are four icons with labels: "Draw Structure", "Upload ID List", "Browse Data", and "Periodic Table".

No campo de busca digitamos *sodium chloride*, como indicado abaixo.

U.S. National Library of Medicine
National Center for Biotechnology Information

PubChem About Blog Submit Contact PubChem Periodic Table and Element pages [Read More >](#)

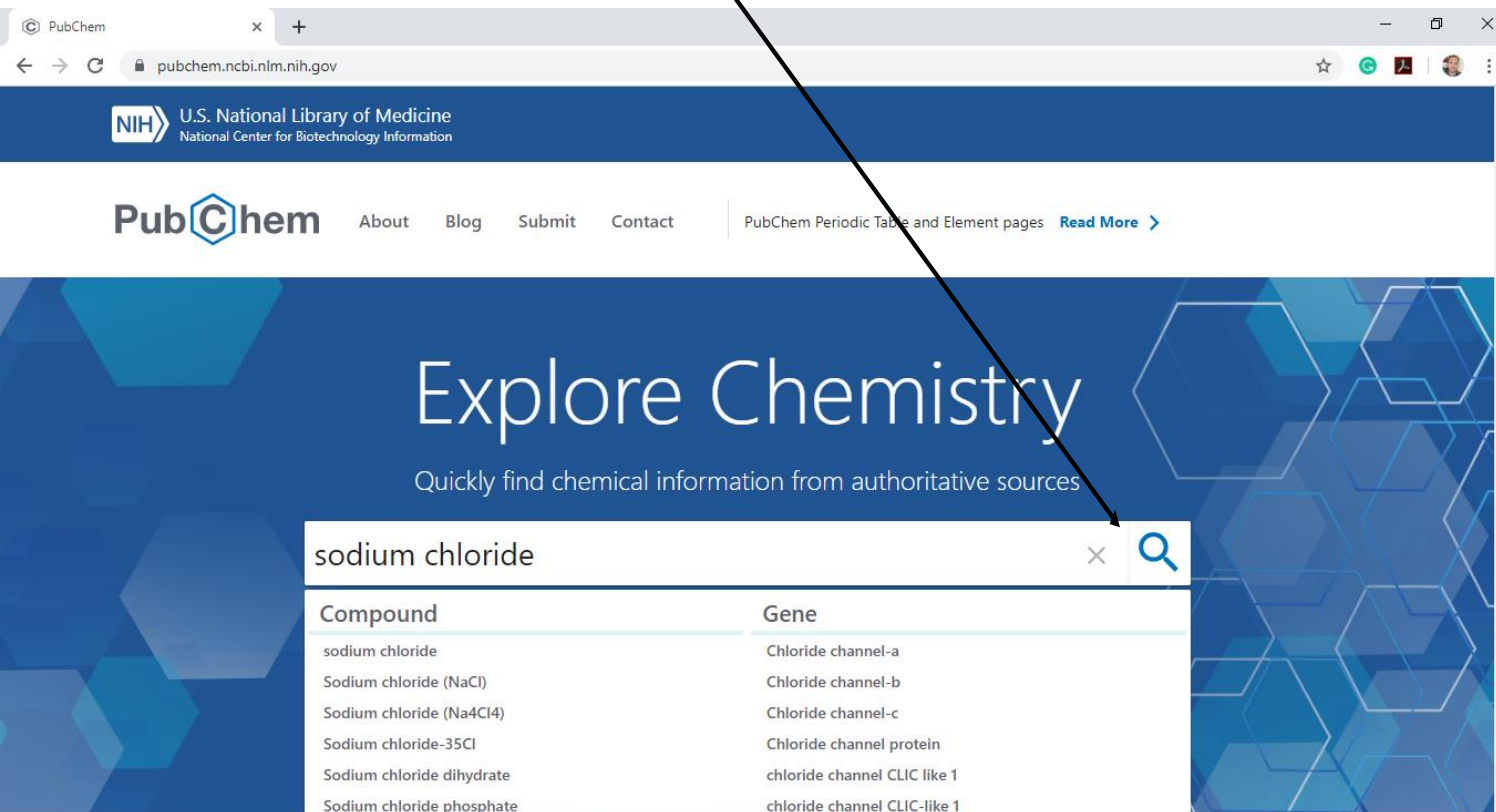
Explore Chemistry

Quickly find chemical information from authoritative sources

sodium chloride

Compound	Gene
sodium chloride	Chloride channel-a
Sodium chloride (NaCl)	Chloride channel-b
Sodium chloride (Na ₄ Cl ₄)	Chloride channel-c
Sodium chloride-35Cl	Chloride channel protein
Sodium chloride dihydrate	chloride channel CLIC like 1
Sodium chloride phosphate	chloride channel CLIC-like 1

Depois clicamos na lupa.



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National Center for Biotechnology Information

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Explore Chemistry

Quickly find chemical information from authoritative sources

sodium chloride

Compound	Gene
sodium chloride	Chloride channel-a
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Sodium chloride-35Cl	Chloride channel protein
Sodium chloride dihydrate	chloride channel CLIC like 1
Sodium chloride phosphate	chloride channel CLIC-like 1

O resultado da busca é mostrado abaixo. Veja que temos 707 resultados para nossa busca. O número elevado de resultados deve-se à variação de fornecedores e nomes similares que apresentam o termo “sodium chloride”.

The screenshot shows a web browser window with the URL `pubchem.ncbi.nlm.nih.gov/#query=sodium%20chloride`. The search bar contains the text "sodium chloride" and a search icon. Below the search bar, it says "Treating this as a text search." The main content area is titled "COMPOUND BEST MATCH" and displays the following information for Sodium Chloride:

- Sodium Chloride; 7647-14-5; Salt; Halite; Table Salt; Saline; Rock Salt; Common Salt; ...**
- Compound CID: 5234
- MF: ClNa MW: 58.44g/mol
- InChIKey: FAPWRFPIFSIZLT-UHFFFAOYSA-M
- IUPAC Name: [sodium:chloride](#)
- Create Date: 2005-03-25

Below this information are links for "Summary", "Similar Structures Search", "Related Records", and "PubMed (MeSH Keyword)".

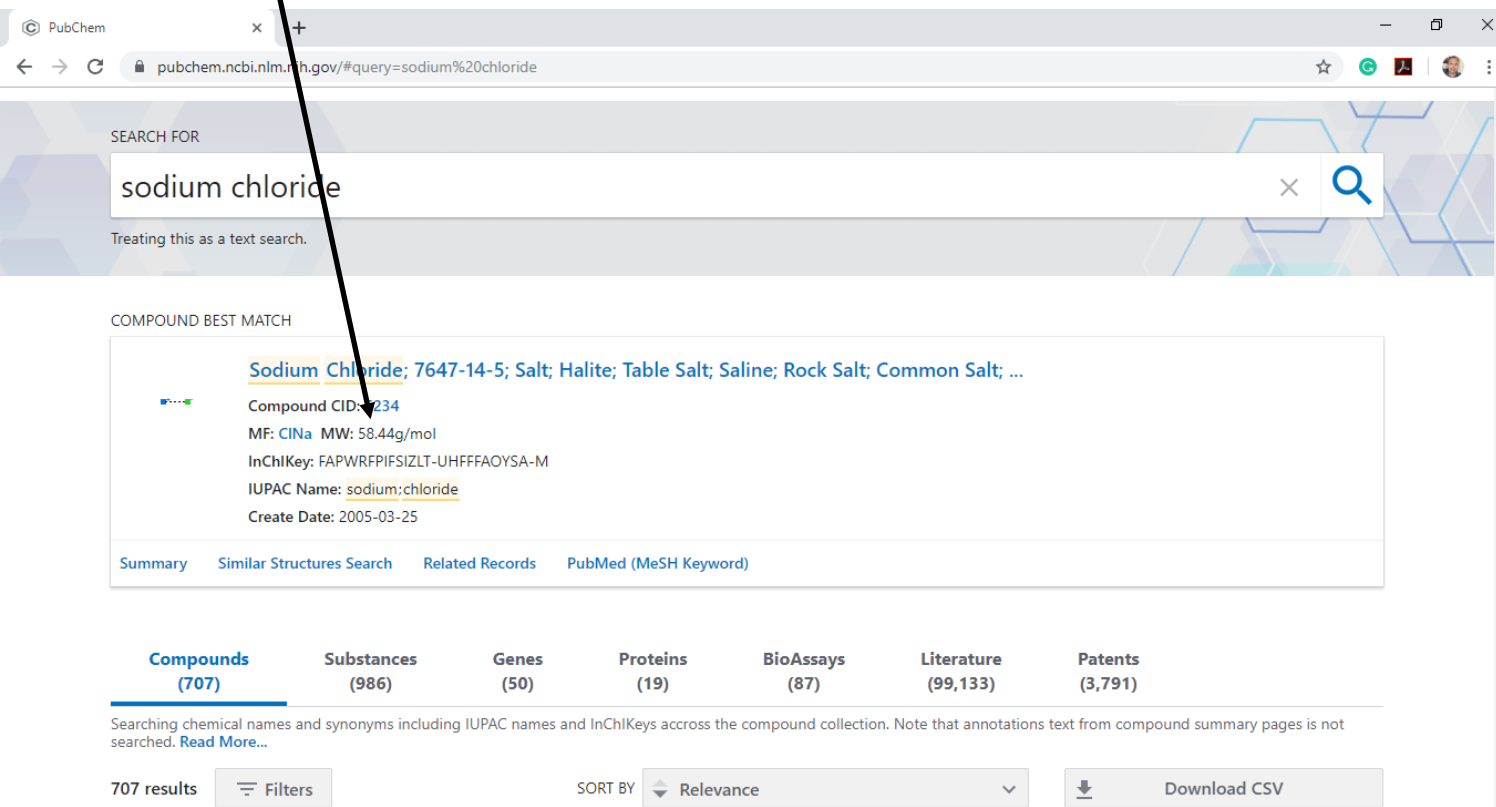
At the bottom of the page, there is a navigation bar with the following categories and counts:

Compounds	Substances	Genes	Proteins	BioAssays	Literature	Patents
(707)	(986)	(50)	(19)	(87)	(99,133)	(3,791)

Below the navigation bar, there is a note: "Searching chemical names and synonyms including IUPAC names and InChIKeys across the compound collection. Note that annotations text from compound summary pages is not searched. [Read More...](#)"

At the bottom of the page, there is a summary bar showing "707 results", a "Filters" button, a "SORT BY" dropdown menu set to "Relevance", and a "Download CSV" button.

Olhando-se o resultado para “sodium chloride”, temos a página abaixo. O conjunto de informações é vasto. Vamos nos concentrar na informação sobre a **massa-fórmula** (*molecular weight*) do cloreto de sódio. O valor da massa-fórmula é 58,44 g/mol.



pubchem.ncbi.nlm.nih.gov/#query=sodium%20chloride

SEARCH FOR
sodium chloride

Treating this as a text search.

COMPOUND BEST MATCH

[Sodium Chloride; 7647-14-5; Salt; Halite; Table Salt; Saline; Rock Salt; Common Salt; ...](#)

Compound CID: [234](#)

MF: [ClNa](#) MW: 58.44g/mol

InChIKey: [FAPWRFPIFSIZLT-UHFFFAOYSA-M](#)

IUPAC Name: [sodium;chloride](#)

Create Date: 2005-03-25

[Summary](#) [Similar Structures Search](#) [Related Records](#) [PubMed \(MeSH Keyword\)](#)

[Compounds \(707\)](#) [Substances \(986\)](#) [Genes \(50\)](#) [Proteins \(19\)](#) [BioAssays \(87\)](#) [Literature \(99,133\)](#) [Patents \(3,791\)](#)

Searching chemical names and synonyms including IUPAC names and InChIKeys across the compound collection. Note that annotations text from compound summary pages is not searched. [Read More...](#)

707 results [Filters](#) SORT BY [Relevance](#) [Download CSV](#)

Aqui cabe uma pequena observação sobre o termo usado em português. Como buscamos informações sobre uma substância iônica (cloreto de sódio) e não molecular, o termo massa molecular não é adequado, assim usamos o termo massa-fórmula. No caso de moléculas, ficamos com o termo massa molecular.

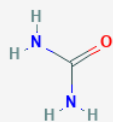
The screenshot shows a web browser window with the URL `pubchem.ncbi.nlm.nih.gov/#query=sodium%20chloride`. The search bar contains the text "sodium chloride" and a search icon. Below the search bar, it says "Treating this as a text search." The main content area is titled "COMPOUND BEST MATCH" and displays the following information for Sodium Chloride:

- [Sodium Chloride; 7647-14-5; Salt; Halite; Table Salt; Saline; Rock Salt; Common Salt; ...](#)
- Compound CID: 5234
- MF: ClNa MW: 58.44g/mol
- InChIKey: FAPWRFPIFSIZLT-UHFFFAOYSA-M
- IUPAC Name: [sodium;chloride](#)
- Create Date: 2005-03-25

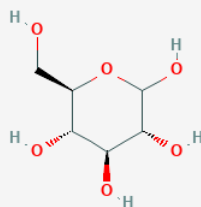
Below this information are several tabs: Summary, Similar Structures Search, Related Records, and PubMed (MeSH Keyword). At the bottom of the page, there are navigation options for different categories: Compounds (707), Substances (986), Genes (50), Proteins (19), BioAssays (87), Literature (99,133), and Patents (3,791). A note at the bottom states: "Searching chemical names and synonyms including IUPAC names and InChIKeys across the compound collection. Note that annotations text from compound summary pages is not searched. [Read More...](#)" At the very bottom, it shows "707 results" with a "Filters" button, a "SORT BY" dropdown menu set to "Relevance", and a "Download CSV" button.

Como exercício, busque informações sobre as substâncias abaixo e anote os valores das respectivas massas moleculares (*molecular weight*).

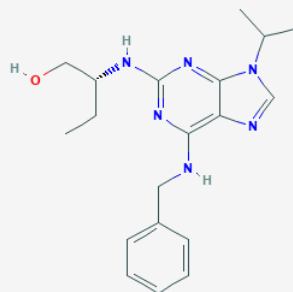
- 1) Ureia (termo em inglês: *Urea*)
- 2) Glicose (termo em inglês: *Glucose*)
- 3) Roscovitina (termo em inglês: *Roscovitine*)
- 4) Ácido acetilsalicílico (termo em inglês: *Acetylsalicylic acid*)
- 5) Captopril (termo em inglês: *Captopril*)



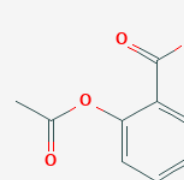
Ureia



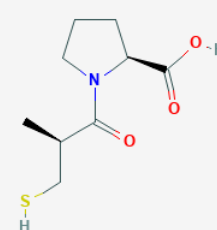
Glicose



Roscovitine



Ácido acetilsalicílico

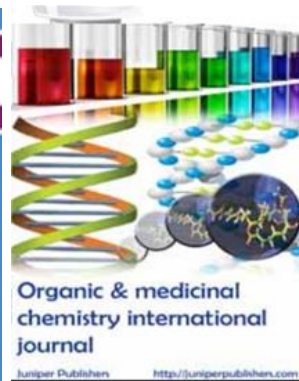
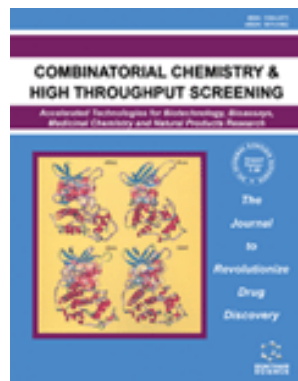
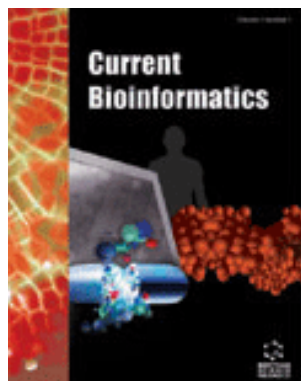


Captopril



Prof. Azevedo is Frontiers Section Editor (Bioinformatics and Biophysics) of the Current Drug Targets, section editor (Bioinformatics in Drug Design and Discovery) of the Current Medicinal Chemistry, section editor (Combinatorial/Medicinal Chemistry) for the Combinatorial Chemistry & High Throughput Screening, member of the editorial board of Current Bioinformatics, and editor of Docking Screens for Drug Discovery (Methods of Molecular Biology)(Springer Nature). He is also member of the editorial board of PeerJ, PeerJ Physical Chemistry, Organic & Medicinal Chemistry International Journal, and section editor in chief (Bioinformatics) of the Bioengineering International. He graduated in Physics (BSc in Physics) from the University of São Paulo (USP) in 1990. He completed a Master Degree in Applied Physics also from the USP (1992), working under the supervision of Prof. Yvonne P. Mascarenhas, the founder of crystallography in Brazil. His dissertation was about X-ray crystallography applied to organometallics compounds (De Azevedo Jr. et al., 1995). During his PhD, he worked under the supervision of Prof. Sung-Hou Kim (University of California, Berkeley), on a split Ph.D. program with a fellowship from Brazilian Research Council (CNPq)(1993-1996). His PhD was about the crystallographic structure of CDK2 (De Azevedo Jr. et al., 1996). His current position is coordinator of the Structural Biochemistry Laboratory at Pontifical Catholic University of Rio Grande do Sul (PUCRS). His research interests are interdisciplinary with two major emphases: molecular simulations and protein-ligand interactions. He published over 190 scientific papers about protein structures and computer models to assess intermolecular interactions involving biomolecules and potential ligands (H-index: 37, RG Index > 41.0). These publications have over 4900 citations in the Web of Science (Publons h-index: 37), more than 5600 citations in the Scopus (h-index: 41), and over 7100 citations in the Google Scholar (h-index: 44).

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<https://www.facebook.com/azevedolab.net/>

The screenshot shows the Facebook profile for 'Azevedolab'. The profile name is 'Azevedolab' with the bio 'Ciência, tecnologia e engenharia em Porto Alegre, Rio Grande do Sul' and 'Sempre aberto'. The page features a navigation menu on the left with options like 'Página inicial', 'Sobre', 'Fotos', 'Website', 'Vídeos', 'Publicações', and 'Comunidade'. The main content area displays a 'Fotos' section with a large schematic flowchart titled 'Schematic Flowchart for Application of Bioinformatics Tools to Discover Drugs Against COVID-19'. The flowchart details a process starting from 'Protein Structures of SARS-CoV-2' and 'Selection of Targets of SARS-CoV-2', moving through 'Machine Learning' (involving IC50 and 3D Structures), 'Molecular Docking', 'Virtual Screening' (using ZINC database), and 'Selection of the Best Hits (Potential New Drugs Against COVID-19)'. It also mentions 'Protein-Ligand Binding Affinity Databases' and 'MOAD'. Below the flowchart are three smaller images: a book cover 'TOP DOWNLOADED PAPER 2018-2019' by Walter Filgueira de Azevedo, Jr., a 'CHEMICAL BIOLOGY & DRUG DESIGN' book cover, and a movie poster for 'ALIEN'. The right sidebar shows 'Comunidade' with 97 likes and 97 followers, and 'Sobre' with a map of the location and contact information for Pontifical Catholic University of Rio Grande do Sul (PUCRS).

Waiting for static.xx.fbcdn.net...

National Center for Biotechnology Information. PubChem Database. Aspirin, CID=2244, <https://pubchem.ncbi.nlm.nih.gov/compound/Aspirin> (accessed on Apr. 20, 2020)

National Center for Biotechnology Information. PubChem Database. Captopril, CID=44093, <https://pubchem.ncbi.nlm.nih.gov/compound/Captopril> (accessed on Apr. 20, 2020)

National Center for Biotechnology Information. PubChem Database. D-Glucose, CID=5793, <https://pubchem.ncbi.nlm.nih.gov/compound/D-Glucose> (accessed on Apr. 20, 2020)

National Center for Biotechnology Information. PubChem Database. Seliciclib, CID=160355, <https://pubchem.ncbi.nlm.nih.gov/compound/Seliciclib> (accessed on Apr. 20, 2020)

National Center for Biotechnology Information. PubChem Database. Urea, CID=1176, <https://pubchem.ncbi.nlm.nih.gov/compound/Urea> (accessed on Apr. 20, 2020)